11º Encontro Nacional de Química-Física

BOOK OF ABSTRACTS

FCUP | SPQ

THEORETICAL STUDY OF EXCITON MIGRATION IN POLYMER--BASED SOLAR CELLS

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Organic solar cells (OSC) are one of the most promising green technologies for energy harvesting. In these devices the active layer is composed of an organic blend of two polymers or by low weight molecule and a polymer. In either case, due to the nature of the materials used, especially of the polymer, the blend morphology at nanoscale strongly affects the main optoelectronic processes that govern OSC functioning. Polymer chains tend to twist and bend, forming nanodomains of conjugated segments with different lengths, which can present different orientations relative to each other and the surrounding medium. Atomistic calculations suggest that the nature of these conjugated segments can affect exciton and charge dynamics in the organic bulk. The dependence of the molecular properties of the conjugated segment on its length dictates the energetic disorder inside the organic network, while the distribution of conjugated segments with different lengths and orientations affects the spatial disorder (see Figure 1). In this communication we will unravel the effect of energetic and spatial disorder in polymer-based solar cells functioning, namely on exciton migration, which is a crucial mechanism on the performance of OSC. To perform our study, we developed a multi-scale model that uses, as input parameters, the results obtained from atomistic calculations, and consider the main physical processes that mediate exciton migration. The model presented here, establishes a clear link between polymer morphology at nanoscale and its influence on exciton migration, which is a breakthrough compared to other computational models published in the literature.

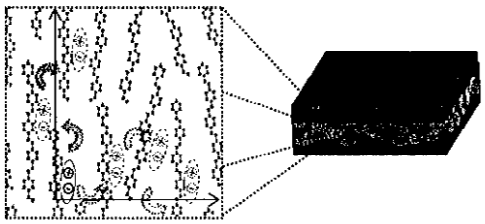

Figure 1 – Schematic representation of exciton migration mediated by conjugated segment orientation in space.

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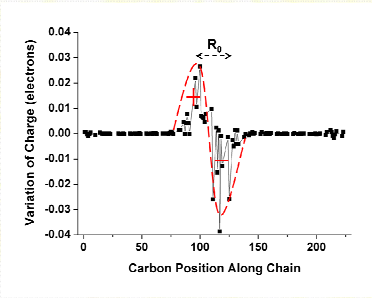
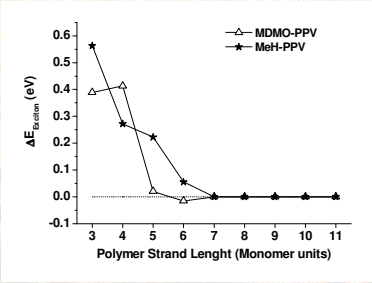
Organic solar cells (OSC) are one of the most promising green technologies for energy harvesting. In these devices the active layer is composed of an organic blend of two polymers or by low weight molecule and a polymer. In either case, the molecular organization at nanoscale strongly affects the main optoelectronic processes that govern OSC functioning. In order to unravel the effect of energetic and spatial disorder in polymer-based solar cells functioning, namely on exciton migration, we developed a multi-scale model that uses, as input parameters, the results obtained from atomistic calculations, and consider the main physical processes that mediate exciton migration. Our results establishes a clear link between polymer morphology at nanoscale and its influence on exciton migration.

ATOMISTIC LEVEL

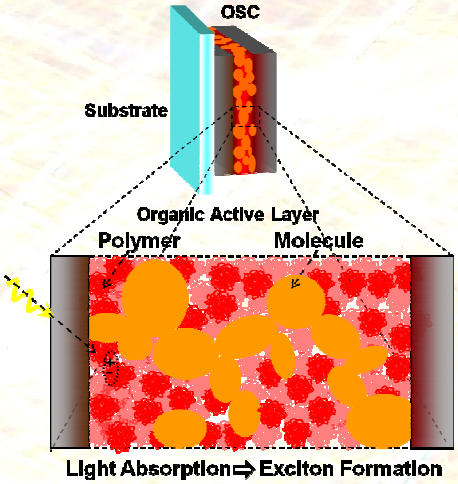
1. Intramolecular Singlet Exciton



2. Energy Barrier Height For Exciton Hopping



MULTI-SCALE MODEL

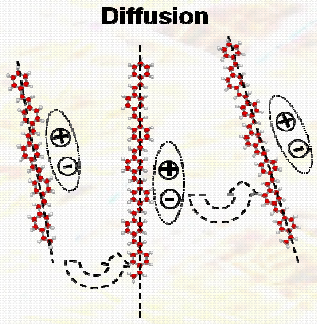


•CHEMOS code (based on a Quantum MD method) was used to extract energy and atomic charge distribution of lowest singlet excited state in conjugated polymer strands.

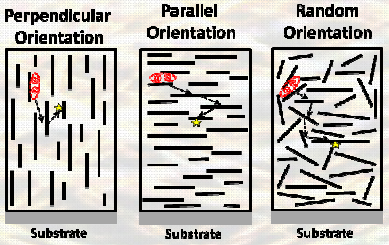
• PHOTO code (based on a Monte Carlo method) was used to simulate exciton migration in polymer networks with different morphologies .

MESOSCPOPIC LEVEL

1. Exciton Hopping



2. Different Polymer Strand Orientation



RESULTS AND CONCLUSION

• Excitons migrate from short conjugated segments (high energy levels) towards longer conjugated segments (lower energy sites).

• The maximum number of exciton decays occurs in conjugated segments with the same length for the two PPV derivatives studied.

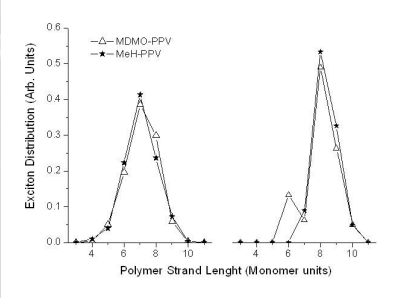


Table 1 – Calculated exciton diffusion length in PPV derivatives.

Conjugated segment orientation.	MDMO-PPV	MEH-PPV
Perpendicular	3.360	3.870
Parallel	4.727	5.546
Random	5.630	6.310

Table 2 – Percentage of physically trapped excitons in PPV derivatives.

Conjugated segment orientation	MDMO-PPV	MEH-PPV
Perpendicular	13.77 %	7.53 %
Parallel	9.70 %	4.43 %
Random	7.27 %	3.57 %

• The orientation of the polymer strands influence the average distance that excitons migrate during their lifetime.

• Different polymer strands orientations creates different distribution of hopping sites and consequently different distributions of dead ends (physical traps) that limit exciton motion.

• Correia, HMG , et. al., Comput. Mater. Sci. 75 (2013) 18-23

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